

On an immersed boundary technique for modeling 3D incompressible fluids laden particles

André S. Müller¹, Eduardo M. B. Campello², Henrique C. Gomes²

¹*Dept. of Civil Construction, Federal Institute of Maranhão*

Av. Getúlio Vargas, 04, 65030-005, São Luís, Brazil

andre.muller@ifma.edu.br

²*Dept. of Structural and Geotechnical Engineering, Polytechnic School, University of São Paulo*

Av. Prof. Almeida Prado, Lane 3, 380, 05508-010, São Paulo/SP, Brazil

campello@usp.br, henrique.campelo@usp.br

Abstract. This work presents results from a recently developed three-dimensional immersed boundary technique for modeling 3D particle-laden fluid problems. A classical Eulerian approach is followed to describe the fluid (assumed here as incompressible through Navier-Stokes equations). A discrete element formulation, in turn, is used to describe the particles' dynamics. The fluid-particle interfaces are treated through Nitsche's method, which is an immersed boundary technique whereby we impose the particles' surface velocities and spins as boundary conditions to the fluid in a weak form. In order to assess the accuracy and efficiency of the developed scheme, numerical simulations of 3D unsteady flow of an incompressible fluid loaded with particles are performed and compared against benchmark solutions. This work refers to an intermediate stage of a scientific research that aims to model problems of fluid-particle interaction (FPI) with full particle-to-particle contacts in particle-laden fluids.

Keywords: particle-laden fluids, fluid-particle interaction, immersed boundary techniques, finite element method, discrete element method.

1 Introduction

The fluid-particle interaction (FPI) subject has great importance in human activities, and it is observed in many phenomena and engineering applications (see e.g. Avci and Wriggers [1] and Johnson and Tezduyar [2]). Basically, if we restrict to numerical point of view, the fluid-particle interface can be handled into two major groups namely, coincident boundary method (see e.g. Donea et al. [3]) and the so-called immersed boundary methods (see Benk, Ulbrich and Mehl [4]).

This work uses the immersed boundary technique to exchange information between these two domains in which, essentially, it considers that the fluid and particle grids are totally independent of each other and overlapped. This work also presents a methodology to simulate the FPI in three-dimensional (3D) space considering the evaluation of the fluid-dynamic forces according to Müller, Campello and Gomes [5] for incompressible fluid flows governed by Navier-Stokes equations. The fluid is defined as an Eulerian description and its discretization is done by a mixed finite element formulation (FEM) within a standard Galerkin framework. The Ladyzhenskaya–Babuška–Brezzi (LBB) compatibility condition (see e.g. Wieters [6] and Bruman and Fernández [7]) is satisfied by using Taylor-Hood tetrahedral elements (Taylor and Hood [8]). The numerical instability, due to convective-dominated problems, is avoided by considering low to moderate Reynolds number even though the Streamline-Upwind Petrov–Galerkin (SUPG) technique is implemented in our code, but we prefer not to introduce this additional complexity here as to keep the focus of the work on the methodology for computation of the FPI. Newmark scheme (Newmark [9]) is adopted for the time integration technique. This is combined with the Lagrangian Discrete Element Method (DEM) for the particle, in our case, spherical particle. The fluid-dynamic

forces and moments represents the influence of the fluid on the motion of the particle and imposed on the latter in a coupled, iterative way. In turn, the influence of the particle on the fluid is considered as a fluid-particle interface problem arising due the use of immersed boundary technique, where the fluid boundary conditions over the particle interface are imposed through Nitsche' method (Nitsche [10]). An explicit and iterative coupled FEM-DEM scheme is developed to achieve convergence within each time step of the solution process. Finally, we present Combined Continuum and Discrete Model (CCDM) to validate the method and illustrate its potentialities to the modeling of particle-laden fluid problems.

This work reports only partial results from broader research, in which we are developing a numerical framework to deal with 3D FPI problems in particle-laden fluid flows where the particle-to-wall (i.e., fluid's exterior solid boundaries) and particle-particle contacts are fully permitted and resolved.

2 The fluid problem

Considering an incompressible viscous fluid governed by Navier-Stokes equations for steady-state problems, we have

$$\rho(\nabla \mathbf{u})\mathbf{u} = \operatorname{div} \mathbf{T} + \rho \mathbf{b} \quad \text{in } \Omega, \quad (1)$$

$$\operatorname{div} \mathbf{u} = 0 \quad \text{in } \Omega, \quad (2)$$

where (1) is the well-known conservation of linear momentum of a material point of the fluid and (2) follows from the mass conservation principle. Above, ρ , \mathbf{u} , \mathbf{T} and \mathbf{b} are the fluid's density, velocity field, Cauchy stress field and volumetric force per unit mass, respectively, with Ω as the problem domain. For an Eulerian description and a Newtonian constitutive law for the fluid, the following system arises from (1) and (2):

$$\begin{aligned} (\nabla \mathbf{u})\mathbf{u} - 2\nu \operatorname{div}(\nabla^s \mathbf{u}) + \nabla p &= \mathbf{b} \quad \text{in } \Omega, \\ \operatorname{div} \mathbf{u} &= 0 \quad \text{in } \Omega, \\ \mathbf{u} &= \bar{\mathbf{u}} \quad \text{in } \Gamma_u, \\ \mathbf{T}\mathbf{n} &= \bar{\mathbf{t}} \quad \text{in } \Gamma_t, \end{aligned} \quad (3)$$

where ν is the fluid's kinematic viscosity, $\nabla^s \mathbf{u}$ is the (symmetric) strain rate tensor and p the fluid's kinematic pressure. Vector \mathbf{n} stands for the unit outward normal to the boundary Γ , and $\bar{\mathbf{u}}$ and $\bar{\mathbf{t}}$ are the prescribed traction and velocity vectors, respectively, on the portions Γ_u and Γ_t of Γ . The third and fourth expressions of (3) represent the boundary conditions of Dirichlet (essential) and Neumann (natural) types, respectively.

The weak form of (3) reads

$$c(\mathbf{u}; \mathbf{w}, \mathbf{u})_\Omega + a(\mathbf{w}, \mathbf{u})_\Omega - (\operatorname{div} \mathbf{w}, p)_\Omega + (q, \operatorname{div} \mathbf{u})_\Omega - (\mathbf{w}, \bar{\mathbf{t}})_{\Gamma_t} = (\mathbf{w}, \mathbf{b})_\Omega \quad \forall \mathbf{w}, q, \quad (4)$$

where \mathbf{w} and q are arbitrary test functions for the velocity and pressure fields, respectively. The trilinear and bilinear forms of the convective and viscous terms above are

$$c(\mathbf{u}; \mathbf{w}, \mathbf{u})_\Omega = \int_\Omega \mathbf{w} \cdot (\nabla \mathbf{u}) \mathbf{u} d\Omega \quad \text{and} \quad a(\mathbf{w}, \mathbf{u})_\Omega = \int_\Omega \nabla \mathbf{w} : \nu \nabla \mathbf{u} d\Omega. \quad (5)$$

2.1 Time and spatial discretization

In temporal discretization, the time variable is discretized into time instants t^n , separated by intervals Δt , such that $t^{n+1} = t^n + \Delta t$ is the time instant immediately after t^n . We adopted the Newmark scheme (Newmark [9]) as a numerical method to integrate eq. (4) in time. In this scheme, the acceleration of the fluid at time t^{n+1} can be expressed as

$$\dot{\mathbf{u}}^{n+1} = \frac{1}{\gamma} \frac{(\mathbf{u}^{n+1} - \mathbf{u}^n)}{\Delta t} - \frac{(1 - \gamma)}{\gamma} \dot{\mathbf{u}}^n, \quad (6)$$

where γ is the Newmark's integration parameter, and where superscript notation is adopted to denote the time

instant at which the corresponding variable is referred to. Here, we use $\gamma = 1/2$ in order to archive second-order accuracy in the integration.

For spatial discretization, a standard mixed finite element scheme is applied where the velocity and pressure fields are the primitive variables of the problem and the fluid's domain is discretized with Taylor-Hood tetrahedral elements (see Taylor and Hood [8]). Such elements use quadratic shape functions for the velocity field and linear shape functions for the pressure field, therewith overcoming numerical instabilities (they fulfill the LBB compatibility condition). Accordingly, the finite element approximation can be written as

$$\begin{aligned} \mathbf{u} &\approx \mathbf{N}_u \mathbf{u}_e \quad \text{and} \quad p \approx \mathbf{N}_p \mathbf{p}_e, \\ \mathbf{w} &\approx \mathbf{N}_u \mathbf{w}_e \quad \text{and} \quad q \approx \mathbf{N}_p \mathbf{q}_e, \end{aligned} \quad (7)$$

where \mathbf{N}_u and \mathbf{N}_p are matrices that contain the element's shape functions of the velocity and pressure fields, respectively, and \mathbf{u}_e and \mathbf{p}_e are the vectors that collect the element's nodal degrees of freedom. Inserting eqs. (6) and (7) into the weak form (4), and performing some algebra, we arrive at the discrete weak form of the fluid problem, which in matrix form is given by

$$\begin{cases} \frac{\mathbf{M}}{\gamma \Delta t} \mathbf{u}^{n+1} + \mathbf{C}(\mathbf{u}^{n+1}) \mathbf{u}^{n+1} + \mathbf{K} \mathbf{u}^{n+1} + \mathbf{G} \mathbf{p}^{n+1} = \mathbf{f}^{n+1} + \frac{\mathbf{M}}{\gamma \Delta t} \mathbf{u}^n + \frac{(1-\gamma)}{\gamma} \mathbf{M} \dot{\mathbf{u}}^n, \\ \mathbf{G}^T \mathbf{u}^{n+1} = \mathbf{0} \end{cases} \quad (8)$$

where \mathbf{M} , \mathbf{C} , \mathbf{K} , \mathbf{G} and \mathbf{G}^T are the mass, convective, viscous, gradient operator and divergent operator matrices, respectively. Still in (8), \mathbf{f}^{n+1} is the vector that contains the field forces and boundary conditions. The system of equations (8) is non-linear due to the convective term, and its solution is achieved using a consistent Newton-Raphson scheme for which full quadratic convergence is ensured. For more details about its numerical derivation and implementation, the interested reader is referred to Müller et al. [11] (the two-dimensional version may be found in Gomes and Pimenta [12]).

3 The particle problem

The motion of the discrete solid particles follows a Lagrangian description here. We assume the particles are spherical. Any deformation they experience is presumed to be very small and localized, therefore they can be treated as rigid bodies. The model herein summarized is described in depth in Campello [13] and [14]. Let us consider a system of N_P particles, each one with mass m_i , radius r_i and rotation inertia $j_i = 2/5(m_i r_i^2)$, with $i = 1, \dots, N_P$. The position of a particle will be denoted by vector \mathbf{x}_i , its velocity by \mathbf{v}_i and its spin by \mathbf{w}_i . The rotation vector relative to the beginning of the motion is denoted by $\boldsymbol{\alpha}_i$, whereas the incremental rotation vector is denoted by $\boldsymbol{\alpha}_i^\Delta$. The rotation field here is also parameterized using the Rodrigues rotation vector, instead of the classical Euler rotation vector. For a detailed account of the rotation description, we refer the reader to Campello [15].

From Euler's laws, the following equations must hold for each particle at every time instant t ,

$$m_i \ddot{\mathbf{x}}_i = \mathbf{f}_i^{\text{tot}} \quad \text{and} \quad j_i \dot{\mathbf{w}}_i = \mathbf{m}_i^{\text{tot}}, \quad (9)$$

in which $\mathbf{f}_i^{\text{tot}}$ is the total force vector acting on the particle and $\mathbf{m}_i^{\text{tot}}$ the total moment vector concerning the particle's center. The superposed dots denote time differentiation. The total force $\mathbf{f}_i^{\text{tot}}$ is the sum of the following force contributions

$$\mathbf{f}_i^{\text{tot}} = m_i \mathbf{g} + \mathbf{f}_i^{\text{fl}}, \quad (10)$$

where \mathbf{g} is the gravity acceleration vector, \mathbf{f}_i^{fl} is the fluid dynamic force vector. In the same way, the total moment applied on the particle is given by the sum of the following contributions:

$$\mathbf{m}_i^{\text{tot}} = \mathbf{m}_i^{\text{fl}} \quad (11)$$

where \mathbf{m}_i^{fl} is the moment generated by fluid dynamic force. Detailed expressions for these force and moment contributions will not be reported here for conciseness (see Müller, Campello and Gomes [5]). Numerical time

integration of eq. (9) provides the particles' motion. This is done here through the integration algorithm proposed in Campello [13], which has both implicit and explicit versions. In this work, we adopt the explicit version only, since this work does not consider any sort of particle contact. The integration algorithm will be omitted here.

4 The fluid-particle interaction problem

The main idea of this work is to use the embedded interface concept in order to compute the fluid flow variables at the fluid-particle interface from an Eulerian fixed mesh. To do so, we resort to the Nitsche's method to enforce the interface constraints (Dirichlet boundary conditions) in a weak sense, for treating the mechanical interactions of overlapping meshes, as depicted in Figure 1. One of the greatest advantages of this method is that it does not add new degrees of freedom to the system.

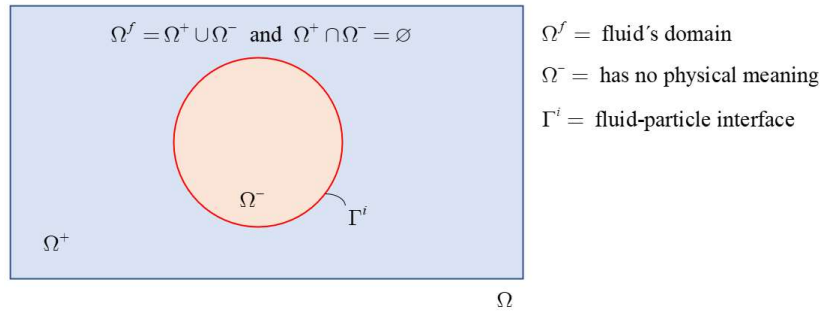


Figure 1. Immersed solid in a fluid and the embedded fluid-particle interface. The interface is discretized into interface elements as to enable the computations. Superscript i stands for the particle's number.

By applying Nitsche's method in (4), after some algebra the discrete weak form in matrix form reads

$$\begin{cases} \frac{\mathbf{M}}{\gamma \Delta t} \mathbf{u}^{n+1} + \mathbf{C}(\mathbf{u}^{n+1}) \mathbf{u}^{n+1} + \mathbf{K}^* \mathbf{u}^{n+1} + \mathbf{G}^* \mathbf{p}^{n+1} = \mathbf{f}^{n+1} + \frac{\mathbf{M}}{\gamma \Delta t} \mathbf{u}^n + \frac{(1-\gamma)}{\gamma} \mathbf{M} \dot{\mathbf{u}}^n + \mathbf{H} \bar{\mathbf{u}}^{n+1}, \\ (\mathbf{G}^*)^T \mathbf{u}^{n+1} = \mathbf{D} \bar{\mathbf{u}}^{n+1} \end{cases}, \quad (12)$$

where

$$\begin{aligned} \mathbf{K}^* &= \mathbf{K} + \mathbf{B} + \mathbf{H}, \mathbf{G}^* = \mathbf{G}_e + \mathbf{D}, (\mathbf{G}^*)^T = \mathbf{G}_e^T + \mathbf{D}^T, \text{ and } \mathbf{H} = \mathbf{B}^T + \mathbf{E} + \mathbf{F}, \\ \mathbf{B} &= \sum_e \mathbf{A}_e^T \int_{\Gamma^i} -\nu \mathbf{N}_u^T [\mathbf{N}_{u,j} (\mathbf{e}_j^T \mathbf{n})] d\Gamma^i \mathbf{A}_e, \mathbf{D} = \sum_e \mathbf{A}_e^T \int_{\Gamma^i} [\mathbf{n}^T \mathbf{N}_u]^T \mathbf{N}_p d\Gamma^i \mathbf{A}_e, \\ \mathbf{E} &= \sum_e \mathbf{A}_e^T \left(\nu \frac{\alpha_1}{h} \right) \int_{\Gamma^i} \mathbf{N}_u^T \mathbf{N}_u d\Gamma^i \mathbf{A}_e \text{ and } \mathbf{F} = \sum_e \mathbf{A}_e^T \left(\frac{\alpha_2}{h} \right) \int_{\Gamma^i} [\mathbf{n}^T \mathbf{N}_u]^T [\mathbf{n}^T \mathbf{N}_u] d\Gamma^i \mathbf{A}_e, \end{aligned} \quad (13)$$

in which h denotes the local mesh size on the boundary Γ^i (or immersed interface) of particle i , α_1 and α_2 are penalty coefficients. The matrix \mathbf{A}_e is the assembling matrix relative to the interface elements of Γ^i . The interested reader is referred to Benk, Ulbrich and Mehl [4] for more details on the Nitsche's method applied to the Navier-Stokes equations.

4.1 Coupled FEM-DEM solution scheme

To compute the time evolution of the system, we follow a time-marching, staggered solution strategy starting from given initial and boundary conditions. At every time step the fluid problem treats the particles as fixed in space, with given positions, velocities and spins. Upon solving for the fluid unknowns (velocity and pressure), the resultant forces and moments on the particles are computed as shown in Müller et al. [5] and passed on the particle problem, which is then solved to obtain the particles' new positions, velocities and spins. The process is then repeated for the next time step until a desired simulation time is achieved. The main steps of the algorithm are

outlined below:

1. Initialize time variables and get initial and boundary conditions.
2. Solve fluid problem at time $t^{n+1} = t^n + \Delta t$ (Newmark integration associated to Newton iterations) considering frozen particles.
3. Compute resultant forces and moment on the particles at time t^{n+1} through Müller et al. [5].
4. Solve particle problem at time t^{n+1} (generalized trapezoidal rule with fixed-point iterations) considering frozen fluid.
5. Update particle fields: positions, velocities and spins.
6. Update time: $t^n \leftarrow t^{n+1}$.
7. Go to step 2.

5 3D Particle sedimentation in a fluid

This example consists of a 3D unsteady fluid-particle interaction. This is a well-known benchmark example in which several experimental results and correlation equation are available. The problem consists of evaluate the particle' terminal velocity, as a result from exact balance between gravity and fluid-dynamic forces. Therefore, a single spherical particle with diameter $d = 5$ cm is released from rest within a narrow recipient filled up with a stagnant fluid, as shown in Figure 2(a). The fluid is governed by the Navier-Stokes equation and its FEM mesh is illustrated in Figure 2(b). The Lagrangian mesh is in Figure 2(c). According to Figure 2(a), only the region referring to the channel core is well refined to reduce the computational cost. The boundary condition of all faces, unless the bottom face, are $(u_1, u_2, u_3) = 0.0$. The convergence tolerance used within the Newton-Raphson iterations is $TOL = 10^{-6}$. Two fluid time steps were analyzed, namely, $\Delta t = 0.005$ s and $\Delta t = 0.0025$ s. In general, the time step of particle is much smaller than that of the fluid. In this case, as there is no collision, the time step of both (fluid and particle) would be the same without loss of precision.

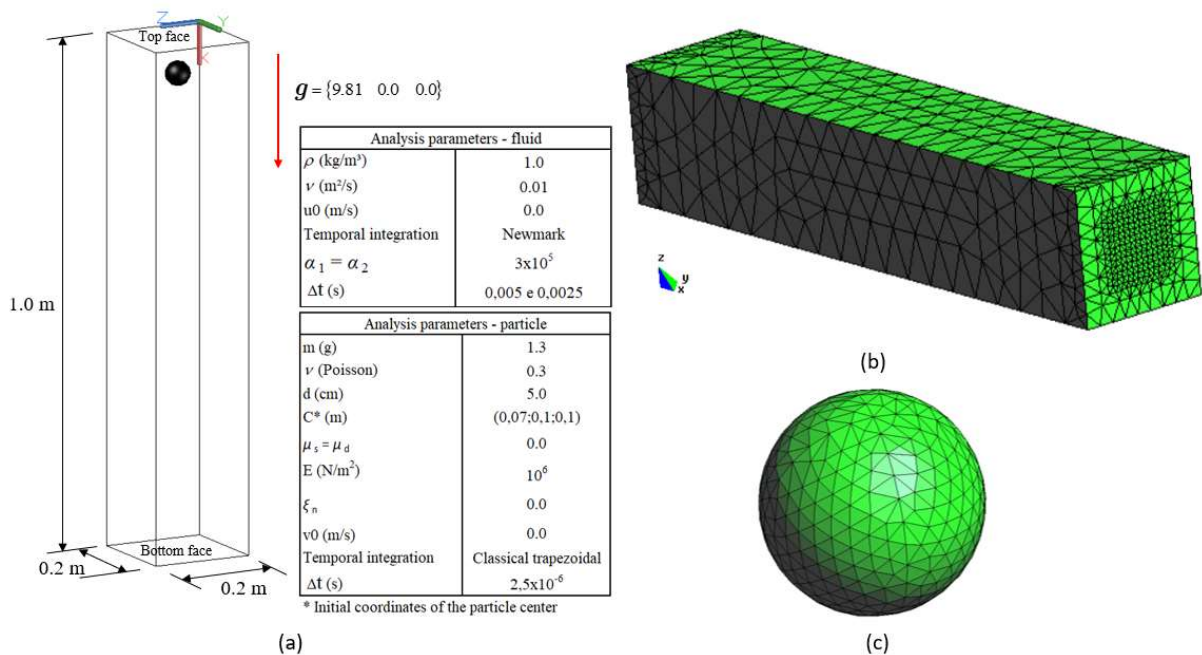


Figure 2. (a) Geometry and analysis parameters of the example 5; (b) Fluid FEM mesh: 158.354 tetrahedral elements and 117.330 nodes; (c) Lagrangian mesh: 780 triangular element and 392 nodes.

Figure 3 shows the results for the time evolution of the velocity field ($\Delta t = 0.005$ s). As we can see, the particle velocity, v_p , is increasing until it reaches approximately 1.60 m/s. After that, the velocity of the particle remains almost the same, characterizing its terminal velocity. We can also note some small transverse displacements (y and z directions) along the channel due, between other reasons, the lack of symmetry of the fluid mesh and the fluid dynamic force in these directions do not be numerically null.

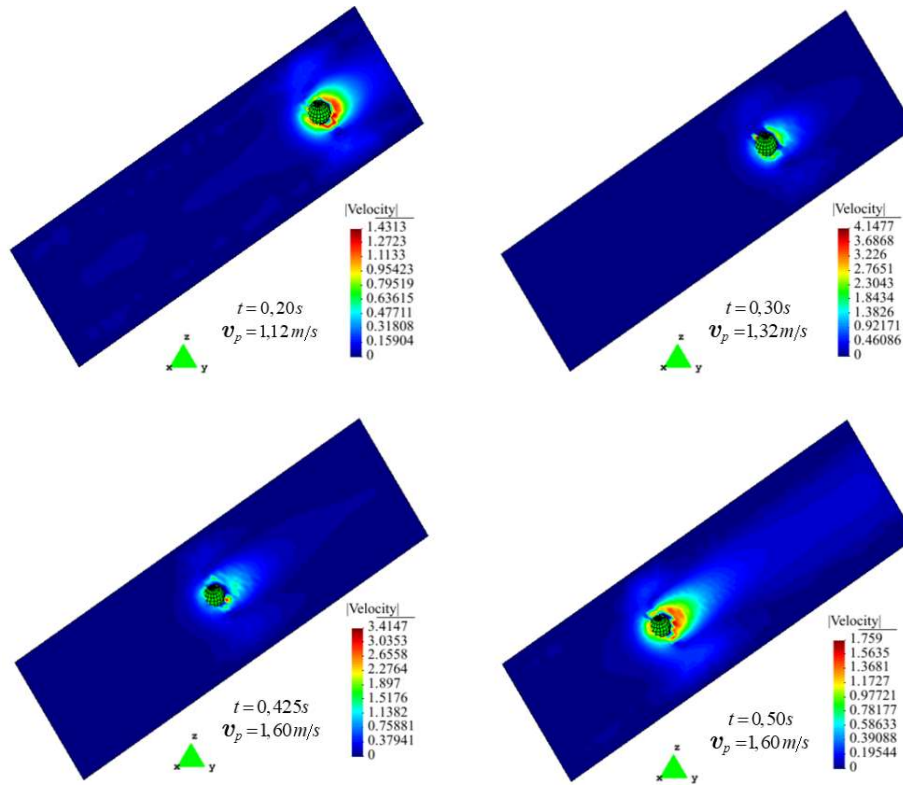


Figure 3. Time evolution of the velocity field.

Figure 4 depicts the graph of the evolution over time of particle velocity. Note that for both cases ($\Delta t = 0.005$ s and $\Delta t = 0.0025$ s) the terminal velocity of the particle is close to the reference values.

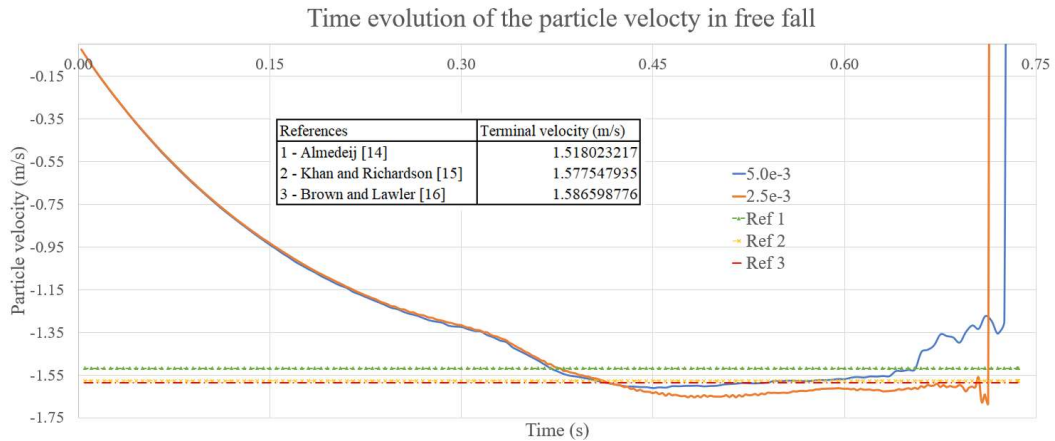


Figure 4. Time evolution of the particle velocity.

6 Conclusions

This work presented a summary of a methodology to simulate the 3D FPI problems. A mixed finite element formulation of an incompressible fluid flow governed by unsteady Navier-Stokes equation was used, along with Nitsche’s method to enforce the Dirichlet boundary conditions in a weak form at the interface. Discrete element method is used to represent the physical behavior of the particle. We showed our first results for 3D simulations using such methodology. We find the present results very promising. A detailed report of this methodology and

its application to other problems, including particle-wall and particle-particle contacts, are the subject of a paper that will be published in a journal in the near future.

Acknowledgements. First author acknowledges support by the Federal Institute of Maranhão, Brazil, and by the Department of Civil Construction. Also acknowledges scholarship funding from FAPEMA (Fundação de Amparo à Pesquisa e ao Desenvolvimento Científico e Tecnológico do Maranhão) under the grant BD-02045/19. Second author acknowledges support by CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico), Brazil, under the grants 307368/2018-1 and 313046/2021-2.

Authorship statement. The authors hereby confirm that they are the sole liable persons responsible for the authorship of this work, and that all material that has been herein included as part of the present paper is either the property (and authorship) of the authors, or has the permission of the owners to be included here.

References

- [1] B. Avci e P. Wriggers, "A DEM-FEM coupling approach for the direct numerical simulation of 3D particulate flows," *Journal of Applied Mechanics*, 2012.
- [2] A. A. Johnson e T. E. Tezduyar, "3D simulation of fluid-particle interactions with the number of particles reaching 100," *Comput. Meth. Appl. Mech. Eng.*, pp. 301-321, 1997.
- [3] J. Donea, A. Huerta, J.-P. Ponthot and A. Rodríguez-Ferran, Arbitrary Lagrangian-Eulerian Methods. In: Stein E, De Borst R, Hughes TJR (eds) Encyclopedia of computational mechanics, New York: Wiley, 2004.
- [4] J. Benk, M. Ulbrich and M. Mehl, "The Nitsche method of the Navier-Stokes equations for immersed and moving boundaries," in *Seventh International Conference on Computational Fluid Dynamics*, Big Island, Hawaii, 2012.
- [5] A. S. Müller, E. M. B. Campello e H. C. Gomes, "A methodology to evaluate fluid-dynamic forces on immersed bodies in 3D fluid flow problems," *XLIV CILAMCE*, 2023.
- [6] C. Wieners, Taylor-Hood elements in 3D. In: Wendland, W.; Efendiev, M. (eds) Analysis and simulation of multifield problems. Lecture Notes in Applied and Computational Mechanics, Berlin: Springer, 2003.
- [7] E. Burman and M. A. Fernández, "Stabilized finite element schemes for incompressible flow using velocity/pressure spaces satisfying the LBB-condition," in *Proceedings of the WCCM VI*, Beijing, 2004.
- [8] C. Hood and P. Taylor, "A numerical solution of the Navier-Stokes equations using the finite element technique," *Computers & Fluids*, pp. 73-100, 1973.
- [9] N. M. Newmark, "A method of computation for structural dynamics," *Journal of the Engineering Mechanics Division*, pp. 67-94, 1959.
- [10] J. Nitsche, "Über ein Variationsprinzip zur Lösung von Dirichlet-problemen bei Verwendung von Teilräumen, die keinen Randbedingungen unterworfen sind," *Abh. Math. Sem. Univ. Hamburg*, pp. 9-15, 1971.
- [11] A. S. Müller, E. M. B. Campello, H. C. Gomes and G. C. Buscaglia, "A numerical method for the three-dimensional simulation of particle-laden fluid flows (in preparation)," *Computer Methods in Applied Mechanics and Engineering*, vol. n/a, p. n/a, 2024.
- [12] H. C. Gomes and P. M. Pimenta, "Embedded interface with discontinuous Lagrange Multipliers for fluid-structure interaction analysis," *International Journal for Computational Methods in Engineering Science and Mechanics*, pp. 1177-1226, 2015.
- [13] E. M. B. Campello, "A computational model for the simulation of dry granular materials," *International Journal of Non-linear Mechanics*, pp. 89-107, 2018.
- [14] E. M. B. Campello, *Um modelo computacional para o estudo de materiais granulares*, São Paulo, 2016.
- [15] E. M. B. Campello, "A description of rotations for DEM models of particle systems," *Computational Particle Mechanics*, pp. 109-125, 2015.